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Abstract

Generalizations of the virial theorem are derived: in atomic physics, in systems including electromagentic radiation, in Newtonian gravitation, and general relativity and also some types of nuclear forces. The cases discussed are limited to potentials which can be produced by the exchange of one particle which include potentials of the form 1/r. The method used is to set equal a change in energy produced by an infinitesimal similarity transformation to a change of energy obtained by a first-order perturbation.

The Simple Virial Theorem in Atomic Structures

A primitive derivation of the virial theorem in atomic physics can be obtained by considering an infinitesimal increase of all masses by a factor $1 + \mu$ (with $\mu << 1$)

$$m \to m\ (1 + \mu)$$

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while leaving all other relevant constants (e, $\hbar$, c) unchanged. A similarity transformation, in which distances (r), momentum values (p), velocities (v), energies (E), and times (t) are replaced by

$$r \rightarrow r\,(1 - \mu)$$
$$p \rightarrow p\,(1 + \mu)$$
$$v \rightarrow v$$
$$E \rightarrow E\,(1 + \mu)$$
$$t \rightarrow t\,(1 - \mu),$$

will leave the Schrödinger equation unchanged. The change in energy μE can be written in terms of potential energy (E_{pot}) and kinetic energy (E_{kin})

$$\mu E = \mu E_{pot} + \mu E_{kin} \quad .$$

The same change in energy may be derived by first-order perturbation which leaves the potential energy which is proportional to e^2/r unchanged, while the kinetic energy p^2/m is perturbed:

$$\frac{p^2}{2m} \rightarrow \frac{p^2}{2m}\,(1 - \mu) \quad .$$

It is to be noted that in first-order perturbation p remains unchanged, while m is changed into m $(1 + \mu)$. Setting equal the change in energy (ΔE) obtained from the similarity transformation and from first-order perturbation we obtain

$$\Delta E = \mu E_{pot} + \mu E_{kin} = -\mu E_{kin}$$

which leads to the most simple form of the virial theorem*

$$E_{pot} + 2E_{kin} = 0 \quad .$$

If the system, which may be macroscopic, is under pressure (P) and is confined to a volume ($V \sim r^3$) then in the similarity transformation the volume will change as

$$V \to V\,(1 - 3\mu) \quad .$$

In this similarity transformation the energy will still change in the same way as above, though the volume is changed. To the previous result of first-order perturbation we should now add the work by the pressure (P) due to the volume contraction ($3\mu V$) which gives

$$\mu E_{pot} + \mu E_{kin} = -\mu E_{kin} + 3\mu PV$$

or

$$E_{pot} + 2E_{kin} = 3PV \tag{1}$$

which is the usual form of the virial theorem. In this equation as well as in the following analogous ones all terms on the left-hand side must be summed or integrated over the components of the system.

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*A similar derivation is based on the variational theorem. If all distances, r, are replaced by $r\,(1 - \mu)$, where μ is infinitesimal, then the change in the potential and in the kinetic energy will be respectively μE_{pot} and $2\mu\, E_{kin}$. According to the variational principle, the sum of these two terms must be zero.[1]

This derivation is valid not only for the actual system but also for the results of approximate calculations such as obtained from the Hartree method, the Thomas-Fermi equation, or the refined form of that equation in which exchange forces are included.[2] It is equally valid in statistical mechanics and can be applied to quasi-ergodic systems which return in a finite time within arbitrarily close limit to any earlier location. In this case the time average of each quantity (E_{pot}, E_{kin}) is considered.

Is the Result of the Similarity Transformation Unique?

Instead of changing m, we may have changed e, $\hbar$, or c. If the latter quantities are changed, however, one should conserve the fine-structure constant $e^2/\hbar c$, otherwise, the nature of our problem will no longer be the same. We shall now show that any of the permissible changes (leaving $e^2/\hbar c$ unaltered) will lead to the same virial theorem.

It is clear that if several of the constants (m, e, $\hbar$, c) are changed by infinitesimal amounts, the results are additive, both in the energy change due to the similarity transformation and in the energy change due to first-order perturbation. Instead of these changes, one may construct another three in which of the three dimensions -- length, time, and mass -- only one changes. We shall now show that of these three only one leads to a non-trivial result: if we change the lengths (r).

It is to be noted that in the discussion given in the first section all three dimensions changed. It is also obvious that if the length (r) is unchanged, the volume (V) will not change and the term 3PV cannot appear.

Furthermore, if the distances and, therefore, the gradients of the wave function remain unchanged, in the wave function of the Schrödinger (or Dirac) equation during the similarity transformation, only the constant (m, e, $\hbar$, c) can be changed. But in the perturbation procedure of the first order the change of the same constants are taken into account exclusively; thus, the two approaches give identical results. Nothing new can be derived.

By contrast if the distances are changed, this has a direct effect on the similarity transformation but not on the first-order perturbation. The perturbation theory is affected only by the change of the constants, while in the similarity transformation both the change of the constants and the change of the variables play a role. In this way only one relation can be derived: the virial theorem.

Magnetic Energy

The virial theorem is applicable in its usual form only to central forces having a $1/r^m$ dependence. We consider in this paper $1/r$ which is derivable from a $1/r$ potential. Magnetic forces between moving charged particles are not central and spin-orbit or spin-spin forces have a different dependence on r. The method used here is, however, readily applicable.

In the similarity transformation currents remain unchanged and the magnetic moments of spins change as $1/m$ and are, therefore, multiplied by $(1 - \mu)$. Since r is also multiplied by $(1 - \mu)$ and since orbit-orbit, spin-orbit, and spin-spin interactions vary as $1/r$, $1/r^2$, and $1/r^3$, respectively, all these interactions change as $(1 + \mu)$, that is like all other energies. The infinitesimal change in energy in the similarity transformation will therefore be

$$\mu E_{pot} + \mu E_{kin} + \mu E_m$$

where E_m is the magnetic energy and E_{pot} is limited to the Coulomb interaction and no externally imposed fields are assumed.

In first-order perturbation theory we must leave r values, gradients and momentum values unchanged but velocities ($\sim$ p/m) and currents change as $(1 - \mu)$ and magnetic moments of spins change in the same way. Therefore, the change in E_m is proportional to $1/m^2$ and can be written as $-2\mu E_m$.

The generalization of Eq. (1) is

$$E_{pot} + 2E_{kin} + 3E_m = 3PV \quad . \tag{2}$$

This equation may be applied to ferromagnets or superconductors.

If external electromagnetic field and potentials are imposed, the usual term 3PV should be replaced by a more involved expression.

One may then apply Eq. (3) to more complicated situations including a plasma held together by external electromagnetic forces (in most of the research on controlled fusion only external magnetic fields are applied). In that case the right-hand side of Eq. (3) is to be replaced by

$$\int P\vec{r} \cdot d\vec{\sigma} + \int \rho_{el} \vec{\mathcal{E}}_{ext} \cdot \vec{r} d\tau + \int (\vec{i} \times \vec{\mathcal{H}}) \cdot \vec{r} d\tau +$$

$$\int [\vec{\nabla} (\mathcal{H}_{ext} \cdot \vec{\mu}_{mag}) \cdot r d\tau \tag{3a}$$

Here the first term is an integral to be taken over the surface of the finite volume to which the virial theorem is applied. The vector $\vec{r}$ is drawn from the surface element over which we integrate to an arbitrary fixed point and $d\vec{\sigma}$ is a vector perpendicular to the surface element and pointing inward; it has the absolute value $d\sigma$. It is easy to see that this integral is equal to 3PV. In the second term, ρ_{el} is the electric charged density and $\vec{\mathcal{E}}_{ext}$ is the electric field imposed by external sources. The vector $\vec{r}$ points from the volume element to a fixed position. In the third term the current density is $\vec{i}$ and $\vec{\mathcal{H}}_{ext}$ is the independently given magnetic field, usually the confining agent acting on the plasma. Finally, the last term is due to the force of the inhomogeneous magnetic field and μ_{mag} is the magnetic moment of the spin. Here the gradient operator $\vec{\nabla}$ is to be applied to the magnetic interaction $(\vec{\mathcal{H}}_{ext} \cdot \mu_{mag})$. All integrations have to be carried out over the volume of the plasma. In experiments involving a high temperature plasma, the pressure, P, is usually zero since the plasma is not supposed to be in contact with the container. The whole right-hand side is the sum of all the forces imposed on the plasma volume under consideration.

The modified form of Eq. (3) can be applied to a part of a system where the left-hand side is summed or integrated over the part of the system under consideration while the right-hand side describes the forces due to all other portions of the whole system. Our approach to the virial theorem would then involve an application of the similarity transformation to the total system. In the perturbation theory the similarity changes still apply to the "external" parts while in the "internal" part only m is replaced by m (1 + μ) and the work accomplished by the motion of the "internal" part relative to the "external" parts must be added. This procedure could be useful in numerical calculations in that more crude zoning may become permissible.

If one wants to verify that application of the virial theorem to parts add up to the virial theorem for the whole system, orbit-orbit, spin-orbit, and spin-spin interactions must be separately considered. For instance, the factor 3 in the term $3E_m$ for the spin-spin case is due to the $1/r^3$ interaction and its influence on the term due to the work considered in our procedure. The other terms in the $3E_m$ expression have a more complex origin.

Electromagnetic Radiation

So far we have included only stationary, or slowly varying, electric and magnetic fields. It seems reasonable that the energy of electromagnetic radiation behaves like the potential energy. This is actually the case.

Indeed, the electromagnetic radiative energy density

$$\frac{1}{8\pi} (\mathcal{E}^2 + \mathcal{H}^2)$$

changes in the similarity transformation like $(1 + 4\mu)$ since $\mathcal{E}$ and $\mathcal{H}$ change due to

$$r \to r \, (1 - \mu)$$

as

$$\mathcal{E} \to \mathcal{E} \; (1 + 2\mu)$$
$$\mathcal{H} \to \mathcal{H} \; (1 + 2\mu) \quad .$$

If we multiply the energy density by the volume element $d\tau$, which changes as $(1 - 3\mu)$ and integrate, we obtain for the electromagnetic radiation energy

$$E_{em} = \int \frac{1}{8\pi} (\mathcal{E}^2 + \mathcal{H}^2)\, d\tau$$

and the similarity change

$$E_{em} \rightarrow E_{em} (1 + \mu) \quad .$$

That is the radiation energy changes like all other energies.

In the perturbation calculation E_{em} remains unchanged.

Therefore, Eq. (2) may be replaced by

$$E_{pot} + E_{em} + 2E_{kin} + 3E_m = 3PV \quad . \tag{3}$$

This equation may be applied to stars in which radiation may account for a considerable fraction of the energy in a steady state (or quasi-ergodic state, i.e., a variable star), though gravitational energy has to be included. This will be done farther below.

Relativistic Equations

If we want to apply our equation to cases where special relativity must be taken into account, the similarity transformation remains unchanged But, in the first-order perturbation calculation E_{kin} and E_m must be reexamined.

For the first of these we may write

$$E_{kin} = [(mc^2)^2 + c^2p^2]^{1/2}$$

where m is the rest mass and mc^2 has been included in E_{kin}. The change in kinetic energy ΔE_{kin} due to an infinitesimal change in m will become

$$\Delta E_{kin} = [((1 + \mu) mc^2)^2 + c^2p^2]^{1/2} - [(mc^2)^2 + c^2p^2]^{1/2} =$$

$$\mu E_{kin} \left(\frac{mc^2}{E_{kin}}\right)^2 .$$

In considering the portion of E_m which is the current-current interaction, this quantity is not simply proportional to $1/m^2$ but to $\left(\frac{c^2}{E_{kin}}\right)^2$. For the change of the relevant part of ΔE_m due to first-order perturbation (where the momentum p is kept constant) we may, therefore, write

$$\Delta E_m = E_m \left[\left(\frac{E_{kin}}{E_{kin} + \Delta E_{kin}}\right)^2 - 1\right] = 2\mu E_m \left(\frac{mc^2}{E_{kin}}\right)^2 .$$

Using the calculated values of ΔE_{kin} and ΔE_m one obtains for the relativistic form of the virial theorem

$$E_{pot} + E_{em} + E_{kin} \left[1 - \left(\frac{mc^2}{E_{kin}}\right)^2\right] + E_m \left[1 + 2 \left(\frac{mc^2}{E_{kin}}\right)^2\right] = 3PV . \tag{4}$$

What has been said so far about the relativistic case relates to macroscopic situations. The most discussed case in quantum mechanics is the Dirac equation for a single particle. Straightforward application of our procedure gives

$$E = mc^2 \overline{\beta} = [(\psi_1|\psi_1) + (\psi_2|\psi_2) - (\psi_3|\psi_3) - (\psi_4|\psi_4)] mc^2$$

where β is the Dirac operator which is positive for the first pair of components and negative for the second pair. The left-hand side is obtained from the similarity transformation while the right-hand side is derived by the perturbation theory where only the term βmc^2 is changed.

If we subtract this relation from the Dirac equation averaged over a stationary state we obtain the more usual form of the virial theorem[1]

$$E_{pot} + c\vec{\alpha} \cdot \vec{p} = 0.$$

Here $c\vec{\alpha}$ stands for the velocity and $\vec{p}$ for the momentum.

One may get a different generalization of the virial theorem by deriving the Klein-Gordon equation from the Dirac equation. For sake of simplicity, this will be done in the absence of magnetic fields. The result is

$$(E - E_{pot})^2 \psi = (p^2c^2 + m^2c^4) \psi \quad .$$

This holds, of course, for any single-particle problem. If the average is taken over a stationary state and if, as is permissible for $E_{pot} \approx \frac{1}{r}$ the change $m \rightarrow m(1 + \mu)$ leads to $E \rightarrow E(1 + \mu)$ then the perturbation theory gives

$$E\,(E - \overline{E_{pot}}) = m^2c^4$$

where $\overline{E_{pot}} = (\psi | E_{pot} | \psi)$. The solution of this equation yields for $\overline{E_{pot}} < 0$

$$E = \frac{1}{2}\,[\overline{E_{pot}} + (\overline{E_{pot}}^{\,2} + 4\,m^2c^4)^{1/2}]$$

where the positive square root should be taken. The reason for this relatively simple result is that the term $\overline{E_{pot}}^2$ dropped out when taking the difference of energies after and before the similarity transformation. This would not have been possible if higher power of $E - \overline{E_{pot}}$ had been taken.

An interesting though bizarre consequence of our potential-theory result is the situation arising if $\overline{E_{pot}}^{\,2} \gg m^2c^4$. In this case the approximate result is

$$E \approx \frac{m^2c^4}{|\overline{E_{pot}}|} \quad .$$

It is obvious that any stable solutions must have a positive energy. For $\overline{E_{pot}}^{\,2} \gg m^2c^4$ it is by no means obvious that stable solutions exist. It may be possible to assume a continuum of such solutions with infinitely many modes near $r = 0$. We see, in addition, that the values of E will be inversely proportional to $|\overline{E_{pot}}|$.

The quantum-mechanical, many-body problem is essentially unsolved. To approximate solutions, like the Hartree method, generalizations of the virial theorem can be applied.[3]

Gravitation and General Relativity

In our derivation of the virial theorem for atomic structures we assumed that the charge of the electron, e, remained unchanged, but we replaced all masses m by $m\,(1 + \mu)$. To retain the argument in the same form we must assume that the gravitational interaction of two masses Gm^2 must not change. Hence, we have

$$G \to G\,(1 - 2\mu) \quad .$$

Designating the potential energy of gravitation by E_{grav} one obtains for isolated systems in the non-relativistic approximation

$$E_{pot} + E_{em} + E_{grav} + 2E_{kin} = 3PV \tag{5}$$

where E_{kin} includes macroscopic as well as atomic and subatomic motions. Nuclear energies are not taken into account and for the sake of simplicity energy E_m is neglected* in Eq. (5). In the obvious applications to stars, globular clusters, and galaxies P = 0 and the right-hand side of Eq. (5) vanishes. The same conclusions also apply to periodic and quasi-ergodic motion such as cepheid variables and rotating stars or galaxies. In this case all terms must be replaced by their time averages.

One can also apply the virial theorem to a part of an astronomical object, for instance, to an arbitrarily defined volume within a star. Then the right-hand side of Eq. (5) will not be zero but will have the form

$$\int P\vec{r} \cdot \vec{d}\sigma + \int (\vec{g}_{ext} \cdot \vec{r}\,)\,\rho d\tau \tag{5a}$$

where the first term becomes 3PV provided the pressure is a constant over the surface which in the present case is not always true. In the second terms g_{ext}, is the gravitational acceleration due to external masses and ρ the density. The integration is to be carried out over the volume.

*Its inclusion would be routine.

It is interesting to note that if a star is subdivided into two regions, an internal sphere and an external shell, then the interaction potentials occur twice. This wrong factor two is corrected when the second term in the expression (5a) is taken into account. Similar considerations apply to Eq. (3a).

The application to general relativity is remarkably simple. Actually the similarity transformation may be used without change.

To see this one has to consider the definition of space curvature. The relevant point is the angular change of a vector carried around an infinitesimal surface in four-dimensional space, divided by the area of that surface. This curvature is proportional to the gravitational constant G and the energy-momentum-tension tensor which is an energy per unit volume. Thus, we get

$$G \frac{E}{r^3} \sim \frac{(1-2\mu)\,(1+\mu)}{(1-3\mu)} = 1 + 2\mu \quad .$$

On the other hand, the angular change of the vector is the curvature times the area since r and t change as $1 - \mu$ the area is proportional $1 - 2\mu$. Thus, the change in the direction remains unaltered by the similarity transformation if the vector is carried around a scaled-down area.

The first-order perturbation theory may be applied in an unchanged fashion. Thus, one is led to the equation for an isolated system

$$E_{pot} + E_{em} + E_{kin}\left[1 - \left(\frac{mc^2}{E_{kin}}\right)^2\right] = E_{pot} + E_{em}\frac{p^2c^2}{E_{kin}} = 0 \quad . \tag{6}$$

In Eq. (6) E_{pot} includes the Coulomb energy as well as all forms of the gravitational energy. We again use $E_{kin}^2 = (mc^2)^2 + c^2p^2$ which leads to the rewriting of the third term in Eq. (6). This term is to be summed over all particles in the isolated systems (star, cluster, or galaxy) under consideration.

If the system is not isolated but is under the influence of external pressure and externally imposed gravitational forces, the right-hand side of Eq. (6) will not be zero but will be of the same form as stated in the case of Eq. (5). It should be recognized, however, that in general relativity there is no obvious way in which to separate out the gravitation forces g_{ext} due to the external masses. Indeed, the solutions in general relativity are supposed to be self-consistent.

All energies should be given the value as seen by one selected observer who is at rest relative to the observed sytem or, in case of periodic motion, relative to the average position of the system. For different observers terms in Eq. (6) will change due to a change of the gravitational red-shift which will amount to a common factor in all terms.

Equation (6) does not apply to black holes, not even to very massive black holes (with a correspondingly big radius) in which high densities such as those occurring in atomic nuclei need not be considered. On the one hand, the interior of a black hole is unobservable. On the other, the formation of a black hole needs infinite time; though configurations closely approaching a black hole can be obtained in a short time, systematic, non-ergodic velocities approaching light velocity are necessarily involved. All our considerations apply only to systems which remain in or return to the same state, at least in good approximation.

Application to Nuclear Forces

There is no indication that forces which increase the separation of the interacting particles such as occur in the description of quarks in quantum chromodynamics can be treated by any method resembling the virial theorem. On the other hand, older theories describing nuclear forces based on the exchange of mesons might be treated in analogy with the procedures used in this paper.

We again perform a similarity transformation in which all masses are changed by a factor $1 + \mu$. These masses include those of the Yukawa particles which are exchanged. The potentials due to these particles are of the Coulomb type with an added exponential factor $e - \frac{r}{r_Y}$ where r_Y is the Yukawa distance and is inversely proportional to the mass of the Yukawa particle. The similarity transformation holds with all masses changed by a factor $1 + \mu$ and all distances changed by a factor $1 - \mu$. The masses include m_Y, the Yukawa mass, and the distances, the Yukawa radius, r_Y, which changes by $1 - \mu$. The result is an equation similar to Eq. (1) except that on the left-hand side a term will appear $\frac{r}{r_Y} E_Y$, where E_Y is the Yukawa potential and r_Y is again the Yukawa radius. In this expression r is the distance between a pair of nucleons and a sum over all the pairs has to be taken.

Actually, several terms of this kind will have to be introduced, depending on various Yukawa masses that can be exchanged between nucleons. In this way Yukawa-type repulsive potentials may be introduced which, of course, have in general a shorter range than the attractive interactions.

The virial theorem can be further generalized to the older approaches of nuclear forces when one introduces orbit-orbit interactions, spin-orbit interactions, and spin-spin interactions or tensor forces. The appearance of these various forces will be simialr to what we discussed in connection with Eq. (3) and in relation to the magnetic term E_m. The discussion here is a simple translation of what has been said in connection with Eq. (3). In every case, the similarity transformation will occur as usual with the only exception being that m_γ and r_γ have to be changed as described. In every case, therefore, additional terms of the form $\frac{r}{r_\gamma} E_\gamma$ will make their appearance where E_γ stands for the various kinds of Yukawa interactions describing plain interactions, orbit-orbit interactions, spin-orbit interactions, and spin-spin interactions. The latter three will furthermore carry a factor 3 as did E_m in Eq. (3).

For clarity we repeat the reasons for their occurrence. Every one of these terms will occur with a factor 1 due to the similarity transformation. In addition, in case of the orbit-orbit interactions perturbation theory will add the term multiplied by a factor 2 due to the perturbation originating from the changed mass of the nucleons which in perturbation theory corresponds at a constant momentum to a decrease of the velocity of the interacting particles. Since, however, it is this velocity which gives rise to the orbit-orbit interaction, the perturbation theory will give a factor $-\mu$ on the right-hand side of the equation which can be transferred to the left-hand side with a positive sign and will furnish two more terms of the orbit-orbit type due to the two interacting particles.

In the case of the spin-orbit and spin-spin type of interactions, the exponential factors are preceded by a $1/r^2$ or $1/r^3$ dependence, respectively. In order to maintain the similarity transformation, the forces due to the spin as well as the forces due to the velocity of the motion have to be reduced by a factor $1 - \mu$. This will result in all cases in a further factor 2μ due to the perturbation theory which will in the end give rise to a factor 3 in analogy with the one obtained for E_m in Eq. (3).

It might be mentioned that the spin-orbit forces have played a particularly strong role in the shell theory of nuclear structure. This is probably due to the circumstance that the spin-orbit forces are strong when the gradients of the potentials become pronounced. The Yukawa-type behavior increases these gradients.

The end result is an expression similar to Eq. (3) in which, however, on the left side Yukawa-type additions of the appearance $\frac{r}{r_Y} E_Y^*$ have to be added for every Yukawa-type force whether it be a simple type interaction or one analogous to the terms designated as E_m in Eq. (3).

It would be tempting to apply these considerations to the interior of neutron stars. This would appear to be possible by using virial-type expressions on volume elements within the neutron star and deriving sound velocities by deriving expressions for $\frac{dP}{d\rho} = \frac{1}{c^2}\frac{dP}{dE}$ where ρ is the mass density and E the energy density. In some approximations, one can see how a sound velocity $\frac{c}{\sqrt{3}}$ is approached; this sound velocity is, indeed, characteristic for ideal gases at very high temperatures.

The appearance of strong repulsive forces and the corresponding Yukawa potentials which can become predominant at high pressures can give rise in a formal sense to velocities higher than the velocity of light. One of my old memories is that Fermi asked me in 1951 or 1952 how probable it was tnat within ten years a velocity would be discovered exceeding light velocity. My answer was one in a million. Fermi then told me he thought it was 10%, the well known value for a Fermi miracle. Unfortunately, I remain convinced that the probability for the next ten years is even now 10^{-6}.

The derivation of sound velocity discussed in previous paragraphs seems actually to be inapplicable for velocities approaching the velocity of light. The expression $\frac{dP}{d\rho}$ is defined in a static way, but is based on the exchange of mesons. The circumstance that these mesons themselves cannot move faster than light should make the derivation based on static compressibilities inapplicable. We seem to have reached in this regard the limits of the usefulness of the methods that are applied in this paper.

*It is noted that these extra terms should in no case be multiplied by a factor 3 since they are obtained from the similarity transformation and no contribution is made by the perturbation theorem.

Conclusion

Many of the results obtained in this paper are repetitions of the obvious. Others approach the absurd. I am deeply indebted to my friend, Mort Weiss, who prevented me from going over the edge and also encouraged me by his interest in what appeared almost obvious. I hope, particularly with his help, to have touched upon some subjects which are neither obvious nor absurd.

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